Supplementary Material

New insight of kinetics study on different loading CuO/CNT catalyst and its optimization for

p-chloroaniline photodegradation

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Equations on mass transfer study

The Thiele Modulus equations used are as follow:

$$\varphi = R_p \sqrt{\frac{k_v}{D_{eff}}}$$

where

R_p is the catalyst size (m),

k_v is an apparent rate constant, and

D_{eff} is the effective diffusion coefficient.

The effective diffusion coefficient can be obtained by equation below:

$$D_{eff} = \frac{\varepsilon}{\tau} D_{AB}$$

where

D_{AB} is the diffusivity (D_{AB}) m²/s

ε is porosity of the catalyst

τ is tortuosity

The diffusivity can be obtained by equation below;

$$D_{AB} = (1.173x10^{-16})(\emptyset M_B)^{1/2} \frac{T}{\mu_B V_A^{0.6}}$$

$$T = 1 - 0.5\ln (1 - \varepsilon)$$

Φ is association parameter of solvent = 2.26

M_B molecular weight of solvent = 18 kg/kmol

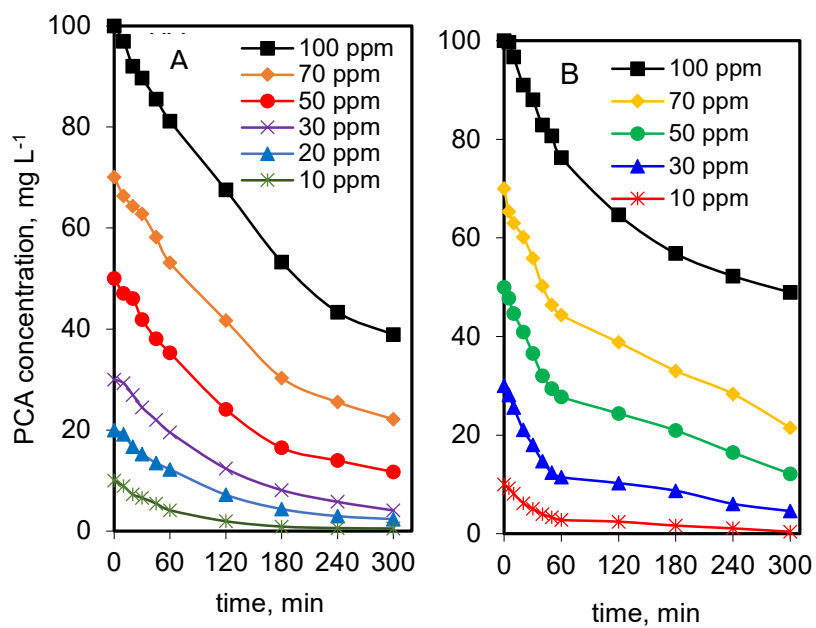viscosity of solution (μ_B) = 0.00089 kg/m-s

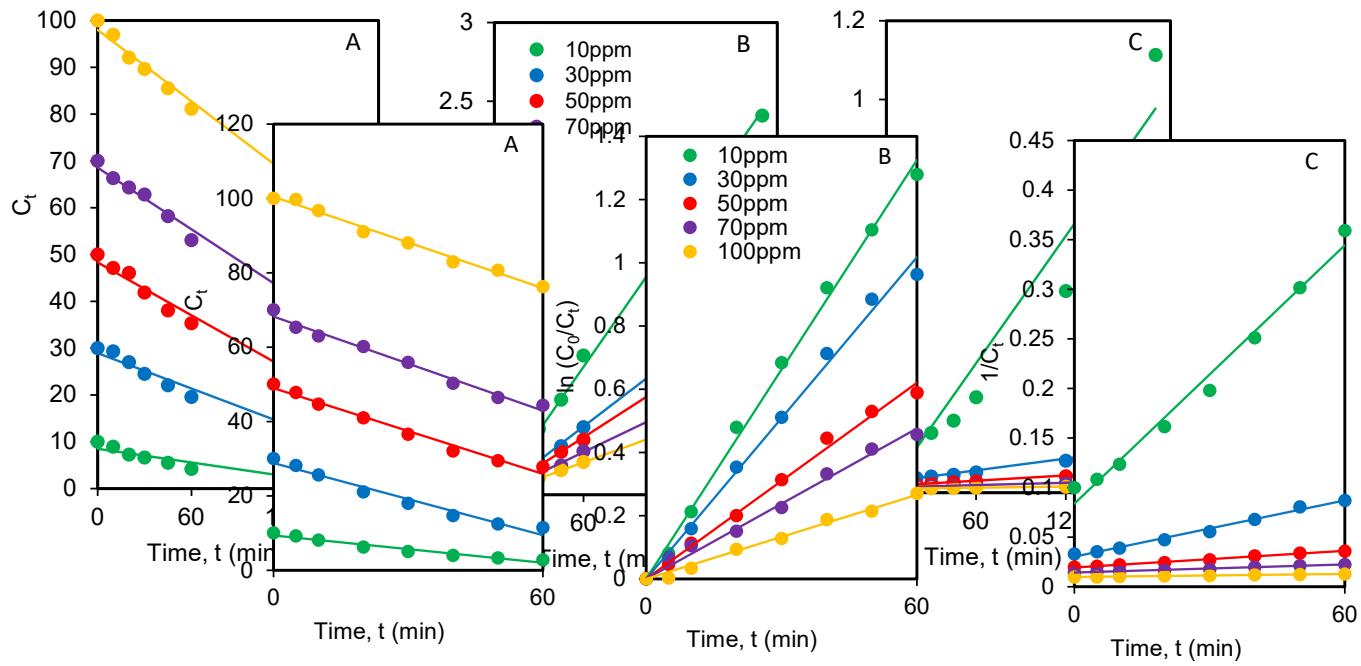Fig S1. Effect of initial concentration for PCA degradation under A) UV and B) VIS irradiation.

Fig S2. The linear plots of A) zeroth-order, B) first-order, C) second-order kinetics models under UV and D) zeroth-order, E) first-order, and F) second-order kinetics model under VIS systems
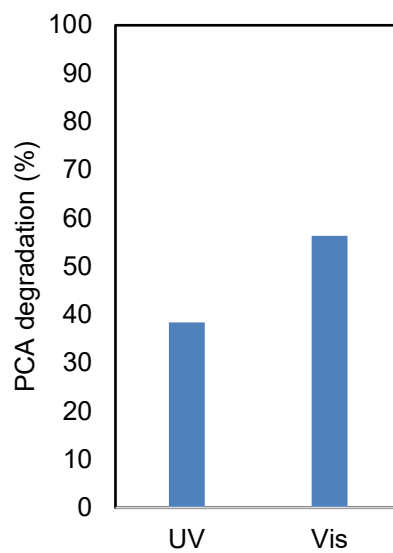
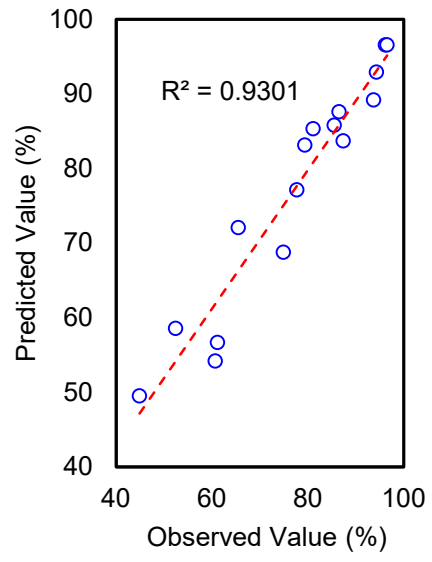Fig. S3. PCA photodegradation performance over TiO$_2$ (Degussa P25) under both systems.

Fig. S4 Parity Chart

Table S1. Apparent rate constant and percentage degradation under UV and VIS light irradiation

	UV light irradiation						
	reaction order						PCA degradation (%)
	zeroth		first		second		
initial concentration (ppm)	$k \times 10^{-2}$ (mol L^{-1}. min^{-1})	R^2	$k \times 10^{-2}$ (min^{-1})	R^2	$k \times 10^{-2}$ (L. mol^{-1}. min^{-1})	R^2	
10	4.87	0.888	1.36	0.998	0.54	0.926	96.3
30	12.6	0.966	0.72	0.997	0.05	0.975	88.1
50	18.8	0.980	0.61	0.998	0.02	0.976	80.3
70	21.9	0.996	0.45	0.993	0.01	0.976	69.4
100	25.4	0.998	0.34	0.992	0.05	0.986	66.2

	VIS light irradiation						
initial concentration (ppm)	reaction order						PCA degradation (%)
	zeroth		first		second		
	$k \times 10^{-2}$	R^2	$k \times 10^{-2}$	R^2	$k \times 10^{-2}$	R^2	
10	12.3	0.998	2.21	0.996	0.43	0.986	96.8
30	32.4	0.995	1.70	0.984	0.09	0.989	84.7
50	38.5	0.993	1.03	0.987	0.03	0.994	75.7
70	42.2	0.970	0.79	0.989	0.01	0.988	69.3
100	41.0	0.955	0.44	0.990	0.005	0.993	51.0

Table S2 Initial rates and photonic efficiency for 2M methanol oxidation

Catalyst	k_{app}, (min^{-1})	Rate, r_0 (mmol L^{-1} s^{-1})	Photonic efficiency, Φ (%)
3 wt% CuO/CNT	0.0132	4.40E-07	0.028
50 wt% CuO/CNT	0.0268	8.93E-07	0.026

Table S3 Experimental design and response value for different conditions

| Run | Independent variables | | | Response (Y) | |
	pH (A)	Catalyst dosage (B)	Initial concentration (C)	Observed	Predicted
1	3	0.125	5	60.7	54.19
2	3	0.125	15	52.4	58.58
3	3	0.625	5	44.9	49.50
4	3	0.625	15	87.4	83.69
5	11	0.125	5	79.4	83.17
6	11	0.125	15	61.2	56.66
7	11	0.625	5	74.9	68.78
8	11	0.625	15	65.5	72.07
9	3	0.375	10	77.7	77.14
10	11	0.375	10	85.5	85.82
11	7	0.125	10	86.5	87.60
12	7	0.625	10	94.3	92.96
13	7	0.375	5	81.1	85.36
14	7	0.375	15	93.7	89.20
15	7	0.375	10	96.2	96.60
16	7	0.375	10	96.5	96.60

Table S4 Analysis of Variance (ANOVA) for Quadratic Model

Sources	Sum of Square (SS)	Degree of Freedom (DoF)	Mean Square (MS)	F-value	$F_{0.05}$
(1) pH (L)	188.356	1	188.3560	4.14069	0.088068
pH (Q)	602.903	1	602.9031	13.25380	0.010827
(2) Catalyst Dosage(L)	71.824	1	71.8240	1.57893	0.255620
Catalyst Dosage(Q)	105.383	1	105.3831	2.31667	0.178818
(3) Initial concentration(L)	36.864	1	36.8640	0.81039	0.402688
Initial concentration(Q)	229.120	1	229.1195	5.03680	0.065958
1L by 2L	47.045	1	47.0450	1.03420	0.348413
1L by 3L	477.405	1	477.4050	10.49494	0.017696
2L by 3L	444.020	1	444.0200	9.76103	0.020473
Residual	272.934	6	45.4891		
Total SS	3906.174	15			